O 5: Organic-inorganic hybrid systems and organic films I

Time: Monday 10:30–13:00 Location: MA 042

Invited Talk O 5.1 Mon 10:30 MA 042

In-situ studies of organic thin films — •Thorsten Wagner — Experimental Physics, Johannes Kepler University Linz, Austria

The performance of electronic devices based on organic thin films,. e.g. LEDs, field effect transistors and solar cells, correlates strongly with the crystalline structure and the morphology of the organic layer. To study the transition of ultrathin films from 2D to 3D growth, Photoelectron Emission Microscopy (PEEM) and Differential Reflectance Spectroscopy (DRS) are applied in situ and in real-time during the deposition of the molecules. The PEEM provides local information on the wetting layer and on μm sized crystallites with a lateral resolution in the 100 nm range. In spectroscopic mode, the electronic density of states is accessible like in conventional UPS but with a much better resolution. The application of linear polarized light for the excitation of the photoelectrons makes the PEEM also sensitive to the in-plane orientation of the molecules. DRS compares the reflectivity of the bare surface to the one of the surface after deposition of molecules. Due to the different environment of the molecules in the first, the second, and higher layers, these layers can be easily identified based on their spectral fingerprints. For anisotropic samples, linear polarized light (pol-DRS) can be used to obtain information about the orientation of the molecules. The combination of both techniques, applied synchronized in one experiment, turns out to be a very powerful tool to make a direct correlation of the morphology and the optical properties of the sample. As an example, the deposition of α-sexithiophene on different silver surfaces will be discussed throughout the entire presentation.

O 5.2 Mon 11:00 MA 042

Momentum resolved electronic structure of the endo-fullerene Sc3N@C80 on Ag(111) — •Christina Schott[1], Norman Haag[1], Johannes Seidel[1], Leah L. Kelly[1], Mirko Cinchetti[2], Benjamin Stadtmüller[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [2]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund, Germany

Single molecular magnets (SMM) are highly promising materials to reduce the lateral dimensions of magnetic data storage units to the molecular limit. Here, we aim to disentangle the electronic coupling of the organic and the spin carrying part of SMMs and metallic surfaces. As model system, we have chosen the endo-fullerenes Sc3N@C80 for which the atomic spin centers are encased by a robust carbon cage. For a bulk-like film of Sc3N@C80 on Ag(111), we combine momentum resolved photoemission and photoemission tomography to assign the emission features of the molecular orbitals to characteristic parts of the SMM, i.e., to the carbon cage or the atomic spin centers. Spectroscopic differences between the bulk-like film and a Sc3N@C80 monolayer film on Ag(111) can hence be directly linked to the electronic coupling of these molecular parts and the surface. Our results will provide novel insight into the coupling mechanism of spin centers of SMM with (ferromagnetic) metal surfaces and how it influences the properties of spin centers.

O 5.3 Mon 11:15 MA 042

Photoemission study of the spin transition of Fe(phen)2(SCN)2 films on Au(111) — Johannes Stöckl[1,2], •Benito Arnoldi[1,2], Juliusz A. Wolny[1], Volker Schünemann[1], Benjamin Stadtmüller[1,2,3], and Martin Aeschlimann[1,2] — [1]Dept. of Physics, University of Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kl, Ger — [2]Research Center OPTIMAS, Erwin-Schrödinger-Str. 46, 67663 Kl, Ger — [3]Graduate School Materials Science in Mainz, Erwin-Schrödinger-Str. 46, 67663 Kl, Ger

Spin-crossover (SCO) complexes are highly desirable materials for next generation molecular spintronic applications since their electrical, magnetic and optical properties can be controlled by an external stimuli like light or temperature. Here we use angle resolved photoemission electron spectroscopy (ARPES) to investigate the valence band structure of thin films of the prototypical SCO complex Fe(phen)2(SCN)2 on Au(111) for the diamagnetic low spin (LS) as well as the paramagnetic high spin (HS) state. We identify the spectroscopic fingerprints of the HS and LS state by direct comparison of the PES data recorded at room temperature as well as at 40K. In the LS state at LT, the intensity and energetic position of the HOMO-peak of the SCO materials is clearly different compared to the HS state at RT. The magnitude of the observed changes, i.e., the size of the energy shift, strongly dependents on the thickness of the film. Crucially, we show that optical excitation with CW as well as fs light sources can be used to restore the spectroscopic signature of the HS state after the temperature induced transition, i.e., to induce the LS-HS transion.

O 5.4 Mon 11:30 MA 042

Novel 2D Spinterface: Co-TPT/T4PT networks on metallic surfaces — •Lu Lyu[1], Benito Arnoldi[1], Sina Mousavion[1], Sebastian Becker[1,2], Johannes Stöckl[1], Maniraj Mahalingam[1], Benjamin Stadtmüller[1,3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern — [2]Department of Chemistry, TU Kaiserslautern — [3]Graduate School Materials Science in Mainz, Kaiserslautern

Metal-organic networks are highly flexible hetero-structures consisting of atoms which are linked by organic molecules. Most interestingly, the lateral hybridization between the metallic centers and the organic linker molecules can mediate an indirect coupling between the metallic centers which can lead to collective spin phenomena in these systems. Here, we investigated the geometric and spin-dependent electronic properties of various cobalt based metal-organic networks on cobalt and copper surfaces using LEED, LT-STM and spin-resolved ARPES. As linker molecules, we have chosen the organic molecules TPT (2,4,6-triphenyl-1,3,5-triazine) and T4PT (2,4,6-tri(4-phenyl)-1,3,5-triazine). Upon deposition of these molecules on bare Cu(111) and on thin Co film on Cu(111), metal-organic networks instantaneously formed due to the large amount of free surface adatoms. The Cu-TPT network on Cu(111) reveals single atom cavities which can be filled by Co atoms in an additional deposition step. A comparison between our structural and spin-dependent spectroscopic data will allow us to gain insight into the interactions between the metal atoms and the organic molecules in these networks.

O 5.5 Mon 11:45 MA 042

Towards tailoring the electronic structure of ferromagnetic surface alloys by absorption of organic molecules — •Johannes Seidel[1], Dominik Jungkenn[1], Sina Mousavion[1], Markus Franke[2], Leah L. Kelly[1], Lu Lyu[1], Hans-Joachim Elmers[3], Christian Kumpf[2], Mirko Cinchetti[4], Martin Aeschlimann[1], and Benjamin Stadtmüller[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, D-67663 Kaiserslautern — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, D-52425 Jülich — [3]Institut für Physik, Johannes-Gutenberg-Universität Mainz, D-55122 Mainz — [4]Experimentelle Physik VI, Technische Universität Dortmund, D-44221 Dortmund

In this work, we extend our recent investigations [1] of organic adsorbates on surface alloys to the lanthanide-noble metal surface alloy Dy_1Ag_2/Ag(111). This 2D alloy is highly interesting due to the likely existence of a ferromagnetic phase at low sample temperature [2]. We present a detailed characterization of the electronic structure of the bare Dy_1Ag_2/Ag(111) surface alloy by momentum microscopy. The geometric structure is characterized by STM, LEED and NIXSW. We are able to identify Dy-Ag hybrid states and to reveal a significant vertical buckling of the Dy atoms. Upon the adsorption of PTCDA on Dy_1Ag_2, we find a clear change in the band surface of the surface alloy. These findings will be discussed in the light of the geometric modification of Dy_1Ag_2 surface as well as our previous findings for other surface alloys [1]. [1]PRL**117**, 096805(16); [2]Nano Lett. **16**, 4230(16)

O 5.6 Mon 12:00 MA 042

Band Formation at the Tetraazaperopyrene/Au(111) Interface — •Arnulf Stein[1], Benjamin Günther[2], Lutz H. Gade[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg — [2]Anorganisch-Chemisches Institut, Universität Heidelberg

For the performance of organic semiconductor based (opto)electronic devices the properties of organic/inorganic interfaces play a crucial role. A new class of polyheterocyclic aromatics are the 1,3,8,10-tetraazaperopyrenes (TAPPs) which have already shown to be promising organic semiconductors for applications [1-2]. We studied TAPP-derivatives adsorbed on Au(111) using energy- and angle-resolved two-photon photoemission spectroscopy (2PPE). We determined the electronic structure and observed band formation at the TAPP/Au(111) interfaces.

[1] Martens, S. C. *et al.*, Chem. Eur. J. 18, 3498-3509 (2012).

[2] Hahn, L. *et al.*, Chem. Eur. J. 17691-17700 (2015).

O 5.7 Mon 12:15 MA 042

Structural and electronic phase transition at a metal-organic interface

— •Patrick Amsalem[1,2], Luca Giovanelli[2], Oliver Hofmann[3], Georg Heimel[1], Ahmed Khalladi[4], Norbert Koch[1,5], Tobias Rüffer[4], Thierry Angot[2], and Jean-Marc Themlin[1] — [1]Humboldt-Universität zu Berlin & IRIS Adlershof — [2]Aix-Marseille Universit́e — [3]Graz University of Technology — [4]Technische Universität Chemnitz — [5]Helmholtz-Zentrum Berlin

The performance of hybrid organic-inorganic devices strongly depends on the interface properties such as the organic / electrode interface. In this context, large research efforts have been devoted to understand the phenomena occurring at interfaces formed between large pi-conjugated molecules and metal surfaces. If much progress has been achieved, the effect of the interplay between molecule-metal and intermolecular interaction on the interface electronic properties is not well-documented yet. Here, we address the structural, vibrational and electronic properties of a long-range ordered sub-monolayer film of octachloro zinc-phthalocyanines (ZnPcCl8) adsorbed on Ag(111), which undergo a structural transition consisting mostly in a decrease of the lattice parameters upon gentle annealing (350 K). The vibrational spectra for the two investigated structural phases reveal strong differences in their electronic properties. In addition, monitoring the change in the valence band features allows to correlate the vibrational features with the amount of charge transfer, as well as with the metallic or insulating character of the hybrid interface.

O 5.8 Mon 12:30 MA 042

On-Surface Synthesis of Heptacene and its Interaction with a Metal Surface

— •Malte Zugermeier[1], Manuel Gruber[2], Martin Schmid[1], Benedikt P. Klein[1], Lukas Ruppenthal[1], Philipp Müller[1], Ralf Einholz[3], Wolfgang Hieringer[4], Richard Berndt[2], Holger F. Bettinger[3], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [3]Institut für Organische Chemie, Eberhard Karls Universität Tübingen, Germany — [4]Lehrstuhl für Theoretische Chemie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Acenes are important molecular organic semiconductors, whose electronic properties scale with the length of the conjugated system. With increasing length, the HOMO-LUMO gap and the reorganization energy decrease, while the charge carrier mobility increases. These changes, which are potentially beneficial for applications in organic electronics, are accompanied by unfavorable trends such as increased light sensitivity, increased reactivity towards oxygen, and a higher tendency to form dimers. Therefore, the existence of the larger heptacene was controversial for several decades. We report the on-surface synthesis of heptacene from a diketone precursor on Ag(111) and show that heptacene is stabilized by the presence of the surface. The surface-assisted reaction was monitored by XPS and STM. NEXAFS and DFT provide additional insights into the orientation and the surface interaction of the molecules.

O 5.9 Mon 12:45 MA 042

Metal-Phthalocyanines on Noble Metal Surfaces: A Systematic Investigation With Respect to Strong Correlation Effects

— •Manuel Grimm, Dennis Hein, Christian Metzger, Martin Graus, Achim Schöll, and Friedrich Reinert — Exp. Physik 7, Universität Würzburg, 97074 Würzburg, Germany

Metal-organic interfaces provide an ideal playground to study fundamental interaction mechanisms. In particular cases, these can lead to electronic correlations which cannot be described within a single particle picture. In case of some adsorbate/substrate combinations the LUMO of molecules in the first layer is partially occupied due to charge transfer from the metal substrate. As a result such samples, e.g. NTCDA or CuPc on Ag(111) [1,2] show a sharp Kondo resonance at the Fermi energy in high resolution photoelectron spectroscopy (PES) experiments. Here we present a systematic study of these resonance features. We analyze the influence of sample temperature and vary the bonding strength and charge transfer at the interface by changing the adsorbate and the orientation of the substrate surface. While we observe a Kondo scenario for NiPc and CuPc on Ag(111) which is explained within a Single Impurity Anderson model (SIAM), a more complicated behavior occurs on Ag(100) and Ag(110) surfaces. In the latter cases the NiPc and CuPc LUMO is still partially filled at room temperature, but starts to shift to larger binding energies upon cooling. This also leads to a shift of the sharp resonance peak away from the Fermi energy, which demands for an explanation beyond the SIAM.

[1] Schoell *Science* 329, 303 (2010) [2] Ziroff *PRB* B85 (2012)